# CHEMICAL-MATERIAL COMPATIBILITY STUDY WITH INITIAL DECON GREEN FORMULATION

Philip W. Bartram, Monicia R. Gibson, Vikki D. Henderson
Edgewood Chemical Biological Center
Aberdeen Proving Ground, MD 21010

## ABSTRACT

The army is currently developing Decon Green, a thorough decontaminant intended to be more effective, environmentally friendly, applicable to an extreme temperature range, and more material-compatible than the standard decontaminant DS2. The objective of this study was to compare the effects of Decon Green on thermoplastics and rubbers of military interest with the effects caused by DS2. These effects were observed by comparing physical properties of test specimens before and after exposure to both decontaminants. Percent weight gain, percent extraction, solubility corrected for extraction, rate of decontaminant sorption, and changes in hardness, appearance and volume were noted. It was found that DS2 affected materials to a greater degree than Decon Green.

## INTRODUCTION

The Applied Chemistry Team and the Advanced Chemistry Team, Edgewood Chemical-Biological Center (ECBC), are developing a decontaminant based on peroxymonocarbonate and propylene carbonate. The decontaminant Decon Green will be used as a thorough decontaminant and will replace the U.S. Army's standard chemical agent decontaminant DS-2. The objective of the program is to develop a decontaminant that is as effective against chemical and biological agents, applicable to an extreme temperature range, material compatible, and more environmentally acceptable than DS-2. The current formulation consists of propylene carbonate (≈72.28 wt %), 50% hydrogen peroxide (≈24.42 wt %), Triton X-100 (0.974 wt %), potassium hydrogen carbonate (0.976 wt %), and potassium carbonate (1.35 wt %). This report documents the initial chemical-material compatibility test with Decon Green.

## EXPERIMENTAL METHODS

### MATERIALS AND CHEMICALS

Propylene carbonate, 50% hydrogen peroxide, Triton X-100, potassium hydrogen carbonate, and potassium carbonate were obtained from Aldrich Chemical Company. DS2, 70% diethylenetriamine, 28% methoxyethanol, and 2% sodium hydroxide, was a laboratory sample. The CB Reference Materials are listed in Table 1.[4, 5, 6]

# Report Documentation Page

*Form Approved*
*OMB No. 0704-0188*



| 1. REPORT DATE | 2. REPORT TYPE | 3. DATES COVERED |
|---|---|---|
| **01 JUL 2003** | **N/A** | **-** |

| 4. TITLE AND SUBTITLE | 5a. CONTRACT NUMBER |
|---|---|
| **Chemical-Material Compatibility Study With Initial Decon Green Formulation** | 5b. GRANT NUMBER |
| | 5c. PROGRAM ELEMENT NUMBER |
| 6. AUTHOR(S) | 5d. PROJECT NUMBER |
| | 5e. TASK NUMBER |
| | 5f. WORK UNIT NUMBER |
| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Edgewood Chemical Biological Center Aberdeen Proving Ground, MD 21010** | 8. PERFORMING ORGANIZATION REPORT NUMBER |
| 9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) | 10. SPONSOR/MONITOR'S ACRONYM(S) |
| | 11. SPONSOR/MONITOR'S REPORT NUMBER(S) |

12. DISTRIBUTION/AVAILABILITY STATEMENT
**Approved for public release, distribution unlimited**

13. SUPPLEMENTARY NOTES
**See also ADM001523.**

14. ABSTRACT

15. SUBJECT TERMS

| 16. SECURITY CLASSIFICATION OF: | | | 17. LIMITATION OF ABSTRACT | 18. NUMBER OF PAGES | 19a. NAME OF RESPONSIBLE PERSON |
|---|---|---|---|---|---|
| a. REPORT | b. ABSTRACT | c. THIS PAGE | | | |
| **unclassified** | **unclassified** | **unclassified** | **UU** | **9** | |

Table 1. Materials Exposed to Decon Green and DS2

| SAMPLE | MATERIAL | CODE | SOURCE | USE |
|---|---|---|---|---|
| 1 | Polyethylene methylacrylate acrylic acid | PETA | Smithers Scientific | |
| 2 | Polyethylene propylene | PEP | Smithers Scientific | M40/M42 mask drink tube |
| 3 | Polycarbonate (thermoplastic) | PC | Harbor City Plastics | mask lens |
| 4 | Polybromobutyl isoprene | PBB | Smithers Scientific | M43A1 mask faceblank |
| 5 | Polyurethane | PU | I. B. Moore | |
| 6 | Polyepichlorohydrin | PEH | Smithers Scientific | |
| 7 | Polyvinylchloride (thermoplastic) | PVC | Harbor City Plastics | M24/M25A1 mask |
| 8 | Polyisoprene | PIP | Smithers Scientific | M17A2 /24 /25A1 mask faceblank |
| 9 | Polyphenylene oxide (thermoplastic) | PPO | Harbor City Plastics | M40/42 mask canister component |
| 10 | Polydimethylsiloxane | PDMS | Smithers Scientific | M40/42 mask faceblank |

## PROCEDURE

Three groups consisting of one replicate of each of the above materials were tested. Samples in groups 1 and 2 were immersed in Decon Green at 49$^{o}$C, while Group 3 samples were immersed in DS 2. Samples were removed, blotted and weighed at 15 min and 3 h time intervals. Afterwards, samples were allowed to desorb until their masses stabilized. Measurements (mass, length, width, thickness, hardness) were taken before immersion, at the designated intervals, and after desorption. Changes in appearance were noted throughout.

## CALCULATIONS

Equation 1**:** *Weight gain (WtGn)* = [(wt of specimen + sorbed liquid) - wt of specimen]
Equation 2**:** *Percent weight-gain (%WtGn)* = Wt gain (100) / Wt of dry specimen
Equation 3**:** *Extraction (Ext)* = Wt of specimen - wt of desorbed specimen
Equation 4: *Percent extraction (%Ext)* = Extraction (100) / Initial Wt of specimen
Equation 5**:** *Sorption corrected for Extraction (Scorr%)* = % wt gain + % extraction

# RESULTS AND DISCUSSION

## OBSERVATIONS

Observations on the post-exposure samples are provided in Table 2. When PIP and PBB were immersed in Decon Green, the solution became yellow indicating either a possible chemical reaction or that a component had been extracted from the material; a white residue appeared on the surface of PBB. DS2 and Decon Green either dissolved or degraded polyurethane (PU) within 15 minutes. PPO became tacky after exposure to both Decon Green and DS2. PVC exposed to DS2 changed from creamy white to black. DS2 partially degraded or extracted components from the PDMS sample; however, no degradation or extraction was apparent at the 15-minute weighing. The remaining piece of PDMS was slightly distorted, but pliable.

Table 2. Observations of Chemical-Material Compatibility on Post-Exposure Samples

| SAMPLE | GROUP 1 (Decon Green Exposure) | GROUP 2 (Decon Green Exposure) | GROUP 3 (DS2 Exposure) |
|---|---|---|---|
| PETA | NA | Semi-glossy and tacky | No apparent change |
| PEP | Glossy, smooth and pliable | Glossy and smooth | No apparent Change |
| PC | NA | Dull, cloudy, tacky | Dull, cloudy, tacky. Blue hue changed to violet |
| PBB | Dull, pliable, white residue | White residue, but no residue | No apparent change |
| PU | NA | Dissolved in 15 min | Dissolved in 15 min |
| PEH | Tacky with swelling | Tacky with swelling | Brittle, less pliable. |
| PVC | No apparent change | No apparent change | Color change from white to black |
| PIP | Dull, but no other noticeable changes | Dull, but no other noticeable changes | No apparent change |
| PPO | Tacky | Tacky | Tacky |
| PDMS | No apparent change | No apparent change | Some of material dissolved |

Notes:
NA = not available
49 degrees Celsius for 3 hours and 15 minutes

PERCENT WEIGHT-GAIN

The percent weight-gain for each material in each group and the average for Decon Green replicates at 3 h are provided in Table 3. Decon Green and DS2 either dissolved or degraded PU, and DS2 dissolved PC during the sorption tests. All of the other samples experienced weight gain during the sorption process, except for the PDMS sample exposed to DS2. In most cases, samples exposed to DS2 had a greater percent weight-gain than samples exposed to Decon Green. PEH samples experienced the highest percentage of weight gain among samples in both the DS2 group and the Decon Green group.

Table 3. Percent Weight-Gain for Materials Exposed to Decon Green and DS2

| | GROUP | | | |
|---|---|---|---|---|
| **Material** | **1** (Decon Green Exposure) | **2** (Decon Green Exposure) | **Ave 1 & 2** | **3** (DS2 Exposure) |
| PETA | NT | 27.77 | 27.77 | 18.15 |
| PEP | 0.41 | 0.79 | 0.60 | 1.83 |
| PC | NT | 0.32 | 0.32 | dissolved |
| PBB | 0.70 | 0.88 | 0.79 | 1.84 |
| PU | Dissolved or degraded | Dissolved or degraded | NA | Dissolved or degraded |
| PEH | 49.33 | 51.25 | 50.29 | 91.31 |
| PVC | 0.49 | 0.64 | 0.57 | 4.67 |
| PIP | 0.87 | 1.12 | 1.00 | 5.88 |
| PPO | 0.39 | 0.48 | 0.44 | 0.50 |
| PDMS | 0.55 | 0.29 | 0.42 | -30.72 |

Notes:
NT=not tested
NA= not available
Ave=average
49 degrees Celsius for 3 hours

PERCENT EXTRACTION

The percent extraction values for the materials within each group are provided in Table 4. The average of Group 1 and Group 2 is also provided in Table 4. Most materials exposed to DS2 and Decon Green did not have percent extraction values of more than 2%. The percent extraction values for DS2 samples tended to be negative, indicating that the samples were not fully desorbed, although their masses had stabilized. The samples exposed to Decon Green tended to have positive percent extraction values; indicating that the specimens had either been degraded or components were extracted during the sorption process.

Table 4. Percent Extraction for Materials Exposed to Decon Green and DS2

| | **GROUP** | | | |
|---|---|---|---|---|
| **Material** | **1** (Decon Green Exposure) | **2** (Decon Green Exposure) | **Ave 1 & 2** | **3** (DS2 Exposure) |
| PETA | NT | 4.86 | 4.86 | -5.51 |
| PEP | 0.18 | -0.12 | 0.03 | -1.35 |
| PC | NA | 0.76 | 0.76 | NA |
| PBB | 0.40 | 0.63 | 0.52 | -0.18 |
| PU | NT | NT | NA | NT |
| PEH | 0.79 | 1.62 | 1.21 | -34.14 |
| PVC | -0.09 | -0.21 | -0.15 | -2.08 |
| PIP | 1.18 | 1.72 | 1.45 | -1.91 |
| PPO | 0.02 | 0.01 | 0.02 | -0.04 |
| PDMS | 0.11 | 0.42 | 0.27 | **32.64 |

Notes:
NT=not tested
NA=not available
Ave is average
**PDMS was either partially dissolved or degraded by DS2
49 degrees Celsius for 3 hours

SORPTION CORRECTED FOR EXTRACTION

The sorption-corrected percents for the materials within each group are provided in Table 5. Because each material (excluding PDMS, PC, and PU) exposed to DS2 and PEP (Group 2) and PVC (Groups 1 and 2) had a negative percent extraction, the sorption-corrected percent for those materials is just the percent weight-gain. Typically, sorption-corrected percents were larger for DS2-exposed samples than for Decon Green-exposed samples. The highest sorption-corrected percentages were observed for the PEH samples exposed to either decontaminant.

Table 5. Sorption-Corrected Percent for Materials Exposed to Decon Green and DS2

| | GROUP | | | |
|---|---|---|---|---|
| **Material** | **1** (Decon Green Exposure) | **2** (Decon Green Exposure) | **Ave 1 & 2** | **3** (DS2 Exposure) |
| PETA | NT | 32.63 | 32.63 | 18.15 |
| PEP | 0.60 | 0.79 | 0.70 | 1.83 |
| PC | NT | 1.08 | 1.08 | NT |
| PBB | 1.11 | 1.51 | 1.31 | 1.84 |
| PU | NT | NT | NA | NT |
| PEH | 50.12 | 52.87 | 51.50 | 91.31 |
| PVC | 0.49 | 0.64 | 0.57 | 4.67 |
| PIP | 2.05 | 2.84 | 2.45 | 5.88 |
| PPO | 0.41 | 0.49 | 0.45 | 0.47 |
| PDMS | 0.66 | 0.71 | 0.69 | 1.92 |

Notes:
NT=not tested
NA=not available
Ave =average
49 degrees Celsius for 3 hours

PERCENT CHANGE IN INDENTATION HARDNESS

The percent change in hardness for each material is provided in Table 6. Percent change in hardness values were varied between the two groups of samples exposed to Decon Green; the reason is unknown. The majority of samples from Group 1 experienced negative changes in hardness, indicating that the post-exposure hardness values were less than the pre-exposure hardness values. In contrast, the samples from Group 2 had positive changes in hardness after being exposed to Decon Green indicating that the post-exposure hardness values were greater than pre-exposure hardness values. PDMS from Group 2 had the greatest change, but the initial hardness value of this particular PDMS sample was nearly half the initial hardness value of other PDMS samples. Increases in hardness were observed for PETA, PVC, PIP, PPO and PDMS exposed to DS2. The other Group 3 samples experienced decreases.

Table 6. Percent Change in Hardness for Materials Exposed to Decon Green and DS2

| | GROUP | | | |
|---|---|---|---|---|
| **Material** | **1** (Decon Green Exposure) | **2** (Decon Green Exposure**)** | **Ave 1 & 2** | **3** (DS2 Exposure) |
| PETA | NT | 15.17 | 15.17 | 14.01 |
| PEP | -0.74 | 20.43 | 9.85 | -0.67 |
| PC | NA | 10.21 | 10.21 | NA |
| PBB | -0.45 | 7.37 | 3.46 | -0.28 |
| PU | NT | NT | NA | NT |
| PEH | -2.06 | 12.55 | 5.25 | -53.02 |
| PVC | -0.96 | 7.49 | 3.27 | 7.50 |
| PIP | -0.69 | 26.49 | 12.9 | 27.78 |
| PPO | -1.79 | 5.99 | 2.10 | 6.39 |
| PDMS | -0.56 | 70.24 | 34.84 | 7.29 |

Notes:
NT=not tested
NA=not available
Ave=average
49 degrees Celsius for 3 hours

PERCENT CHANGE IN VOLUME

Both Decon Green and DS2 caused changes in the dimensions of the samples tested. The majority of samples tested with these decontaminants experienced a decrease in overall volume after exposure. The change in volume percentage for each material is provided in Table 7. Every sample tested in Group 1 experienced a decrease in volume except PEP, which had an increase The greatest decrease in volume of Group 1 samples was observed for PBB. PEP and PVC were the only Group 2 samples that had an increase in volume after exposure to Decon Green. The greatest decrease among Group 2 samples was observed for PDMS, which had a volume decrease of ≈30%. In Group 3, only PEH and PVC had positive changes in volume. PEH experienced the greatest increase. PDMS had the largest decrease in volume among samples exposed to DS2.

Table 7. Percent Change in Volume for Materials Exposed to Decon Green and DS2

| | GROUP | | | |
|---|---|---|---|---|
| **Material** | **1** (Decon Green Exposure) | **2** (Decon Green Exposure) | **Ave 1 & 2** | **3** (DS2 Exposure) |
| PETA | NT | -19.90 | -19.90 | -4.08 |
| PEP | 0.59 | 4.90 | 2.75 | -1.50 |
| PC | NA | -1.29 | -1.29 | NA |
| PBB | -22.35 | -23.66 | -23.00 | -21.18 |
| PU | NT | NT | NA | NT |
| PEH | -16.09 | -22.14 | -19.12 | 56.57 |
| PVC | -1.34 | 0.03 | -0.66 | 7.78 |
| PIP | -13.05 | -20.29 | -16.67 | -22.62 |
| PPO | -0.99 | -1.82 | -1.41 | -1.70 |
| PDMS | -22.25 | -29.61 | -25.93 | -41.91 |

Notes:
NT=not tested
NA=not available
Ave=average
49 degrees Celsius for 3 hours

SORPTION AS A FUNCTION OF SURFACE AREA AND TIME

The amount of DS2 and Decon Green sorbed by each material was calculated as a function of surface area per time. The calculations were made for two time intervals, 15 and 180 minutes. The two Decon Green trials (Groups 1 and 2) were averaged together for these calculations. The results are provided in Table 8. The amount of Decon Green and DS2 absorbed by PPO at 15 and 180 minutes, respectively, were similar. The masses of DS2 absorbed by PBB and PEH were approximately twice the amount of Decon Green absorbed by the materials at each time interval. The amount of DS2 absorbed by PEP after 3 h was about 2.5 times the mass of Decon Green sorbed. At 180 minutes, the mass of DS2 absorbed by PVC was a factor of eight greater than the amount of Decon Green absorbed. PIP absorbed more DS2 than Decon Green by a factor of six (t = 180 min).

Table 8. Mass of Decontaminant Absorbed Per Surface Area and Time

| **MATERIAL** | **DECONTAMINANT** | | | |
|---|---|---|---|---|
| | **[a]Decon Green** | | **DS2** | |
| | **μg/cm$^2$ at 15 min** | **μg/cm$^2$ at 180 min** | **μg/cm$^2$ at 15 min** | **μg/cm$^2$ at 180 min** |
| PETA | 2919.5 | 14963.2 | 2276.5 | 9869.7 |
| PEP | 98.7 | 322.7 | 265.6 | 789.5 |
| PC | 281.6 | 340.5 | NA | NA |
| PBB | 146.7 | 425.8 | 266.3 | 945.5 |
| PU | NA | NA | NA | NA |
| PEH | 4338.7 | 32930.4 | 8282.0 | 60612.3 |
| PVC | 302.1 | 683.6 | 913.9 | 5700.5 |
| PIP | 245.3 | 492.7 | 578.4 | 2942.7 |
| PPO | 363.7 | 422.1 | 320.3 | 447.1 |
| PDMS | 103.6 | 144.3 | NA | NA |

Notes:
[a]The Decon Green value is the average of Group 1 and Group 2.
NA=not available

# CONCLUSIONS

Most materials were affected to a greater degree by exposure to DS2 than to Decon Green. DS2 dissolved PC and PU, and partially degraded or extracted PDMS. Decon Green dissolved only PU. Materials exposed to DS2, which were not dissolved or degraded, did not completely desorb even at 70 °C. The only material that did not completely desorb when exposed to Decon Green was PVC. Other materials (PEP, PEH, PVC, PIP) absorbed greater amounts of DS2 than Decon Green. Only PETA absorbed more Decon Green than DS2.

The difference in hardness of the materials after exposure to the two decontaminants is more difficult to evaluate because of inconsistency between Group 1 and Group 2. Typically, the change in hardness was positive for Group 3 (except PEP, PBB, and PEH), Group 2, and the average of Groups 1 and 2.

Typically, materials exposed to DS2 and Decon Green had a negative change in volume. Only PEP (Groups 1 and 2), PEH and PVC (Group 3) had an increase in volume. PEH, PVC, and PDMS when exposed to DS2 had a much larger increase in volume than the samples exposed to Decon Green. Only PETA (Group 2) had a much larger change in volume than PETA exposed to DS2.

Based on the positive trend in the sorption values (Table 8), all materials had not reached equilibrium after 3 h. Therefore, larger exposure times to the decontaminants would cause more severe effects in the materials.

REFERENCES

1. Drago, R. S.; Frank, K. M.; Yang, Yu Chu, and Wagner, G. W., "Catalytic Activation of Hydrogen Peroxide-A Green Oxidant System," Proceedings of the 1997 ERDEC Scientific Conference on Chemical and Biological Defense Research, U.S. Army Edgewood Research, Development, and Engineering Center, Aberdeen Proving Ground, MD, July 1998, UNCLASSIFIED Report (AD-A356-165).
2. Richardson, David E., Yao, Huirong, Drago, Russell S., "Kinetics and Equilibrium Formation of a Weakly Basic Oxidant System for Decontamination," *Proceedings of the 1998 ERDEC Scientific Conference on Chemical and Biological Defense Research*, U.S. Army Edgewood Research, Development, and Engineering Center, Aberdeen Proving Ground, MD, July 1999, UNCLASSIFIED Report (AD-A375-171).
3. Richardson, David E., Huirong Yao, Frank, Karen M., and Bennett, Deon A., "Equilibra, Kinetics, and Mechanism in the Bicarbonate Activation of Hydrogen Peroxide: Oxidation of Sulfides by Peroxymonocarbonates," *J. Am. Chem. Soc*., Vol. 122, pp 1729 – 1740, 2000.
4. Shuely, Wendel J., "Automated Test Methods and Reference Materials for the Selection of Materials for Resistance to Hazardous Chemicals," Lab Automation 2001 Proceedings, Association for Laboratory Automation, University of Virginia, Charlottesville, VA, January 2001.
5. Ince, Brian S., and Shuely, Wendel J., "Interaction of Candidate Cleaning Solutions for Sensitive Equipment Decontamination with Polymeric Materials," *Proceedings of the 2001 Scientific Conference on Chemical and Biological Defense Research, 6-8 March 2001*, U.S. Army Edgewood Chemical-Biological Center, Aberdeen Proving Ground, MD, Oct 2001, UNCLASSIFIED Report.
6. Shuely, Wendel J., "Chemical-Material Compatibility Studies for the NBC Contamination Survivability of Vehicle Materials in the Joint Services Sensitive Equipment Decontamination Program," *NDIA Ground Survivability Proceedings*, March 2001.
7. "Standard Test Method for Resistance of Plastics to Chemical Reagents," *ASTM D 543 – 87 Annual Book of ASTM Standards, Section 8, Plastics*, Vol. 08.01, Philadelphia, PA. 1992.
8. "Standard Test Method for Rubber Property – Effect of Liquids (Attachment 2), *ASTM D 471 Annual Book of ASTM Standards*, Vol. 09.01, West Conshohocken, PA. 1997.
9. Shuely, Wendel J. and Ince, Brian S., *Evaluation of Indentation Hardness Properties and Indentation Methodology for Determining the Influence of Chemical Exposure on Polymeric Materials*, ERDEC-TR-305, U.S. Army Edgewood Research, Development and Engineering Center, Aberdeen Proving Ground, MD, May 1996, Unclassified Report (AD-A310-095).
10. Operation Manual, EXACTA – Hardness Testing System for Rubber, Plastic, and other Non-Metallic Materials, NewAge Industries, Testing Instruments Division, 2300 Maryland Road, Willow Grove, PA 19090.